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Sampling-Theorem Criteria for the Implicit FDTD Methods

Numerical simulations are routinely used for modelling electromagnetic wave propagation problems in the area of high frequency electromagnetics and photonics. The finite-difference time-domain (FDTD) method of explicit type designed by Yee [1] was for long years the preferred numerical technique for such simulations due to its flexibility, since it allows the inclusion of arbitrarily heterogeneous objects in the region to be simulated. In the course of numerical computations artificial artifacts are introduced, such as numerical amplification of the wave power-flow-density (stability issues) as well as the numerical dispersion. For the explicit-type methods the well-known Courant-Friedrichs-Levy (CFL) condition concerning the stability of the calculations must be met, limiting thus the step-length of the in-time-forward-marching algorithm. The extent of literature in this area is huge, including several book publications, e.g. [2].

Recently the implicit types of FDTD methods has been constructed - the "Alternating Directions Implicit" (ADI) FDTD method [3], [4] and the "Crank-Nicholson Split-Step" (CNSS) FDTD method [5], [6]. Both are implicit procedures requiring inversion of tridiagonal matrices in two half-steps. Both are theoretically unconditionally stable, i.e. they enable one to avoid the severe CFL condition and use the unlimited length of the time step in the course of calculation. However, another kind of bounds on the length of the time step, due to aliasing effects with growing time step, is imposed on both these methods.

The Maxwell equations are for the simplicity taken in the simple form for lossless isotropic homogeneous linear medium without external sources, i.e. the permeability μ and the permittivity ε are constants

$$\operatorname{curl}\boldsymbol{H} = \varepsilon\frac{\partial \boldsymbol{E}}{\partial t}, \qquad \operatorname{curl}\boldsymbol{E} = -\mu\frac{\partial \boldsymbol{H}}{\partial t}, \tag{1}$$

where $\boldsymbol{E}(\boldsymbol{r},t)$ and $\boldsymbol{H}(\boldsymbol{r},t)$ are the electromagnetic field intensities for arbitrary time dependence. Writing out (1) into the Cartesian co-ordinate components it yields

$$\varepsilon\frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}, \qquad \mu\frac{\partial H_x}{\partial t} = \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \tag{2}$$

and by cyclic permutation analogously the other four equations.

Maxwell equations are discretised taking so called staggered grids [1] on all three spatial axes and in time with equidistant intervals $\{\Delta_x, \Delta_y, \Delta_z, \Delta_t\}$ (denoted by the serial indexes $\{i, j, m, n\}$), i.e.

$$\begin{aligned}
E_x\left([i+\tfrac{1}{2}]\Delta_x, j\Delta_y, m\Delta_z, [n+\tfrac{1}{2}]\Delta_t\right) &= E_x\Big|_{i+\frac{1}{2},j,m}^{n+\frac{1}{2}} \\
E_y\left(i\Delta_x, [j+\tfrac{1}{2}]\Delta_y, m\Delta_z, [n+\tfrac{1}{2}]\Delta_t\right) &= E_y\Big|_{i,j+\frac{1}{2},m}^{n+\frac{1}{2}}, \\
E_z\left(i\Delta_x, j\Delta_y, [m+\tfrac{1}{2}]\Delta_z, [n+\tfrac{1}{2}]\Delta_t\right) &= E_z\Big|_{i,j,m+\frac{1}{2}}^{n+\frac{1}{2}}
\end{aligned} \tag{3}$$

$$
\begin{aligned}
&H_x\left(i\Delta_x,[j+\tfrac{1}{2}]\Delta_y,[m+\tfrac{1}{2}]\Delta_z,n\Delta_t\right)=H_x\Big|^{n}_{i,j+\frac{1}{2},m+\frac{1}{2}}\\
&H_y\left([i+\tfrac{1}{2}]\Delta_x,j\Delta_y,[m+\tfrac{1}{2}]\Delta_z,n\Delta_t\right)=H_y\Big|^{n}_{i+\frac{1}{2},j,m+\frac{1}{2}}\ .\\
&H_z\left([i+\tfrac{1}{2}]\Delta_x,[j+\tfrac{1}{2}]\Delta_y,m\Delta_z,n\Delta_t\right)=H_z\Big|^{n}_{i+\frac{1}{2},j+\frac{1}{2},m}
\end{aligned}
\tag{4}
$$

Then using the first differences instead of derivatives the discretised equations (2) take the form of explicit equations [1]

$$
\frac{E_x\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,m}-E_x\Big|^{n-\frac{1}{2}}_{i+\frac{1}{2},j,m}}{Z_0c\Delta_t}=\frac{H_z\Big|^{n}_{i+\frac{1}{2},j+\frac{1}{2},m}-H_z\Big|^{n}_{i+\frac{1}{2},j-\frac{1}{2},m}}{\Delta_y}-\frac{H_y\Big|^{n}_{i+\frac{1}{2},j,m+\frac{1}{2}}-H_y\Big|^{n}_{i+\frac{1}{2},j,m-\frac{1}{2}}}{\Delta_z}, \tag{5}
$$

$$
Z_0\frac{H_x\Big|^{n+1}_{i,j+\frac{1}{2},m+\frac{1}{2}}-H_x\Big|^{n}_{i,j+\frac{1}{2},m+\frac{1}{2}}}{c\Delta_t}=\frac{E_y\Big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},m+1}-E_y\Big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},m}}{\Delta_z}-\frac{E_z\Big|^{n+\frac{1}{2}}_{i,j+1,m+\frac{1}{2}}-E_z\Big|^{n+\frac{1}{2}}_{i,j,m+\frac{1}{2}}}{\Delta_y}, \tag{6}
$$

where $c=1\big/\sqrt{\mu\varepsilon}$ is the "physical" propagation velocity in the lossless medium (i.e. the velocity of light) and $Z_0=\sqrt{\mu/\varepsilon}$ is the wave impedance of the lossless medium. The other components are obtained again by the cyclic permutation of the (x,y,z) and (i,j,m) indices.

More than thirty yers later the implicit ADI formulation of the FDTD method appeared [3], [4] which consists in a small modification of e.g. (5) into two substeps where alternately one of the terms on the right side of (5) is taken in the "forward"-layer, i.e. in the first step

$$
2\frac{E_x\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,m}-E_x\Big|^{n}_{i+\frac{1}{2},j,m}}{Z_0c\Delta_t}=\frac{H_z\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},m}-H_z\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j-\frac{1}{2},m}}{\Delta_y}-\frac{H_y\Big|^{n}_{i+\frac{1}{2},j,m+\frac{1}{2}}-H_y\Big|^{n}_{i+\frac{1}{2},j,m-\frac{1}{2}}}{\Delta_z} \tag{7}
$$

and then in the second step

$$
2\frac{E_x\Big|^{n+1}_{i+\frac{1}{2},j,m}-E_x\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,m}}{Z_0c\Delta_t}=\frac{H_z\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},m}-H_z\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j-\frac{1}{2},m}}{\Delta_y}-\frac{H_y\Big|^{n+1}_{i+\frac{1}{2},j,m+\frac{1}{2}}-H_y\Big|^{n+1}_{i+\frac{1}{2},j,m-\frac{1}{2}}}{\Delta_z} \tag{8}
$$

The idea of the CNSS-FDTD method [5], [6] consists in splitting (5) into two half-steps, each in standard Crank-Nicolson formulation, i.e.

$$
\frac{E_x\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,m}-E_x\Big|^{n}_{i+\frac{1}{2},j,m}}{Z_0c\Delta_t}=\frac{H_z\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},m}-H_z\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j-\frac{1}{2},m}}{\Delta_y}+\frac{H_z\Big|^{n}_{i+\frac{1}{2},j+\frac{1}{2},m}-H_z\Big|^{n}_{i+\frac{1}{2},j-\frac{1}{2},m}}{\Delta_y}, \tag{9}
$$

$$
\frac{E_x\Big|^{n+1}_{i+\frac{1}{2},j,m}-E_x\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,m}}{Z_0c\Delta_t}=-\frac{H_y\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,m+\frac{1}{2}}-H_y\Big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,m-\frac{1}{2}}}{\Delta_z}-\frac{H_y\Big|^{n+1}_{i+\frac{1}{2},j,m+\frac{1}{2}}-H_y\Big|^{n+1}_{i+\frac{1}{2},j,m-\frac{1}{2}}}{\Delta_z}. \tag{10}
$$

For the sake of simplicity let us consider the two-dimensional case only. Waves of any temporal and/or spatial shape can be Fourier expanded into the angular spectrum of either TM or TE monochromatic plane waves. Propagation of a spatio-temporal spectral TM component having the vectorial components $\{E_y,H_x,H_z\}$ in the direction given by the k_x, k_z components of the wave vector $\boldsymbol{k}$, $|\boldsymbol{k}|=k=\sqrt{k_x^2+k_z^2}$, is described in two dimensions x and z by

$$
E_y=E_0\exp(j\omega t)\exp(-jk_xx)\exp(-jk_zz), \tag{11}
$$

where the angular frequency ω is given as $\omega = kc = c\sqrt{k_x^2 + k_z^2}$.

The discretised TM plane wave using (11) is given by

$$E_y\Big|_{i,m}^{n} \approx \xi^n \exp(-jk_x\Delta_x i)\exp(-jk_z\Delta_z m), \tag{12}$$

where $\xi = \exp(j\omega\Delta_t)$, and by the similar formulas for $H_x\Big|_{i,m+\frac{1}{2}}^{n+\frac{1}{2}}$ and $H_z\Big|_{i+\frac{1}{2},m}^{n+\frac{1}{2}}$.

However, during the numerical simulation of the wave propagation instead of differential equations the difference equations are being solved. Therefore, instead of the above exact terms, one obtains inexact formula $\xi = \exp(j\omega_A\Delta_t) = \exp(jkv_p\Delta_t)$, where $v_p = \mathrm{phase}(\xi)/k\Delta_t$ is the numerical phase velocity, due to the numerical dispersion different from the "physical" phase velocity *c*. The numerical dispersion, i.e. the differences between *c* and v_p are artifacts stemming from the nature of the numerical procedure itself. To avoid aliasing effects for all discretisations the sampling theorem must be fulfilled, i.e.

$$k_x\Delta_x \le \pi, \quad k_z\Delta_z \le \pi, \quad \omega_A\Delta_t = \mathrm{phase}(\xi) \le \pi. \tag{13}$$

For the ADI-FDTD method using discretised Maxwell equations one obtains for two simulation-half-steps $\Delta_t/2$ the result

$$\sqrt{\xi_{1,2}} = \left(1 + j\sqrt{\left(1 + A_{x,z}^2\right)\left(1 + A_{z,x}^2\right) - 1}\right)\Big/\left(1 + A_{x,z}^2\right), \tag{14}$$

where $A_x = (c\Delta_t/\Delta_x)\sin(k_x\Delta_x/2)$, $A_z = (c\Delta_t/\Delta_z)\sin(k_z\Delta_z/2)$.

For the CNSS-FDTD method one similarly obtains the formula

$$\sqrt{\xi_{1,2}} = \left(2 - A_{x,z}^2 + j2\sqrt{2}A_{x,z}\right)\Big/\left(2 + A_{x,z}^2\right). \tag{15}$$

The power-flow-density for the full step Δ_t is in both cases unconditionally conserved since $|\xi| = \left|\sqrt{\xi_1}\right|\left|\sqrt{\xi_2}\right| = 1$ holds. The dispersion characteristics are fully determined by the phase of $\xi = \sqrt{\xi_1}\sqrt{\xi_2}$ using (14) and (15).

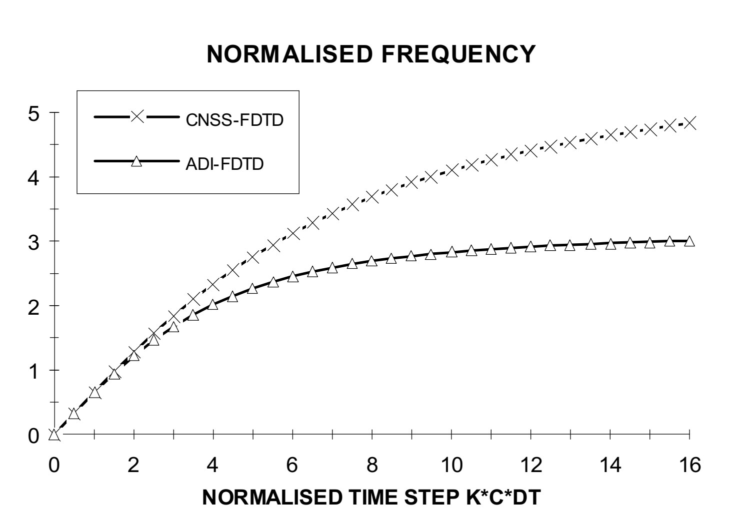

Figure 1. Dependance of the normalised frequency $\omega_A\Delta_t$ on the normalised time step $kc\Delta_t$ for $k_x\Delta_x = 3$, $k_z\Delta_z = 3$.

Wave propagation characteristics using the ADI-FDTD and CNSS-FDTD methods are illustrated in Fig.1. As it can be easily seen the condition (13), i.e. $\omega_A\Delta_t \le \pi$, is fulfilled for CNSS-FDTD until the normalised time step value reaches $kc\Delta_t \approx 6$. For ADI-FDTD it seems that $\omega_A\Delta_t$ reaches the value of π asymptotically. Thus, it can be inferred that the sampling theorem criteria are fulfilled for any step length only for the ADI-FDTD, while for CNSS-FDTD the upper limit $kc\Delta_t \approx 6$ for Δ_t exists. This is a substantial not yet published difference between ADI-FDTD and CNSS-FDTD. Moreover, the arbitrarily long Δ_t step does not necessarily mean any advantage, since with growing Δ_t the phase velocity v_p decreases, i.e. the spatial propagation path pertaining to increased time step remains effectively the same.

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